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# HEAT GRADIENT INDUCED MIGRATION OF BRINE INCLUSIONS IN ROCK SALT
Mathematical treatment

Hans Neltrup

This report has been worked out according to the agreement between Risø National Laboratory and ELSAM/ELKRAFT concerning advisory assistance from Risø to ELSAM/ELKRAFT's waste management project.

Abstract. A mathematical model for the brine migration in rock salt around an infinite line heat source is set up. The temperature field around the time dependent heat source is calculated by use of Green functions. Numerical solutions are obtained by the computer program PSAMA and results are compared with hand calculations for certain simple cases.

By general considerations of the migration field approximate values of the brine inflow, which are independent of the source shape, is obtained and these results are used to estimate the agreement with the experimental results from Project Salt Vault.

INIS descriptors: BRINES, GREEN FUNCTION, MATHEMATICAL MODELS, NUMERICAL SOLUTION, RADIACTIVE WASTE DISPOSAL, ROCKS, SALT DEPOSITS, SPATIAL DISTRIBUTION, TEMPERATURE DEPENDENCE, THERMAL DIFFUSION.

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## 1. INTRODUCTION

The storage of heat producing radioactive waste in rock salt, will produce thermal gradients around the waste depository.

Natural occurring salt formations contain small quantities - typical 0.5 volumen percent brine inclusions with diameters in the range of a few hundred μ's. These inclusions will undergo a migration along the thermal gradient, which in case of pure brine inclusions is directed towards increasing temperature, whereas inclusions containing a gas or vapour buble suspended in the brine will move towards decreasing temperature.

The brine migration thus has two aspects. The first is the inflow of pure brine into the repository. The second is the hypothetical generation of gas or vapour filled inclusions on the wall of the storage hole and their subsequent migration away from the repository, possibly carrying radioactive matter along.

## 2. FORMULATION OF MIGRATION LAW

In ref. (1) and (2) a thorough derivation is given of formulas for the speed with which different types of brine inclusions move.

The present treatment is mainly concerned with the mathematical treatment of the time dependent problem of the brine migration under influence of the decreasing heat production in the waste.

A general expression for the velocity vector, $\vec{V}$ of the brine inclusion which covers formula (10) in ref. (1) and formulas (12) and (13) in ref. (2) may be written as

$$\vec{V} = D_o(T)\nabla T - \frac{K_o}{T} \frac{\nabla T}{\nabla T} \qquad (2.1)$$

where T is the salt temperature.

The first term is an ordinary diffusion term and will in most cases be sufficient to describe the migration. The second term will only be different from zero for drops of pure brine in which case it will only be important for very small drops - order of 10 μ's - and then only as long as it is less or equal to the first term, equality signifying that migration has stopped for this size or smaller drops. For drops containing vapour or gas bubles $K_o = 0$ and $D_o < 0$.

## 3. GEOMETRY FORMULATOR

In order to make the problem tractable it is necessary to assume a one-dimensional temperature field e.g. cylindrical or spherical. Since the waste is supposed somehow to be deposited in drilled holes the present treatment is directed exclusively towards cylindrical symmetry.

Under this symmetry the temperature field is merely a function $T(r,t)$ of the time, t and the distance, r from the axis. If $T(r,t)$ is a known function (2.1) reduces into a simple first order differential equation

$$\frac{dr}{dt} = D_o(T(r,t)) \frac{dT}{dr} - \frac{K_o}{T(r,t)} = f(r,t) \qquad (3.1)$$

The further treatment of this equation depends on which of the two aspects we are considering. If we want to follow the migration of a brine-gas or vapour inclusion we solve (3.1) directly with the initial condition $r(t_o)=r_o$ where $r_o$ is the radius of the storage hole and $t_o$ is the time at which we assume the brine inclusion is generated on its walls.

In case we wish to calculate the amount of brine which has entered the storage hole at a given time $t_o$ after the deposition of the waste, it is practical to calculate backward from the start condition $t=t_o$ and $r=r_o$. By the variable transformation $t=t_o-s \rightarrow \frac{dr}{dt} = -\frac{dr}{ds}$ (3.2) is transformed into

$$\frac{dr}{ds} = -f(r,t_o-s) \tag{3.2}$$

When (3.2) is solved with the initial condition $r(s)=r_o$ for $s=0$ the value $r(t_o)$ will indicate tnat all brine inclusions - assuming same size - inside this radius have crossed the wall of the storage hole.

## 4. CALCULATION OF THE TEMPERATURE FIELD

The temperature field can be expressed on relatively closed form, if the waste cylinders are represented by a time dependent line source $q(t)$

$$T(r,t) = \int_0^t q(\tau)\, \frac{1}{4\pi\lambda}\, \frac{1}{(t-\tau)} \exp\left(-r^2/(4k(t-\tau))\right)d\tau$$

$$= \frac{1}{4\pi\lambda}\int_0^t q(t-\tau)\, \frac{1}{\tau} \exp\left(-r^2/(4k\tau)\right)d\tau \tag{4.1}$$

Here $\lambda$ is the thermal conductivity and $k=\lambda/(c_p\cdot\rho)$ the thermal diffusivity and $c_p\cdot\rho$ the heat kapacity of the salt per unit volume.

By differentiation of (4.1) we get

$$\frac{dT}{dr} = \frac{-r}{8\pi\lambda k}\int^t q(t-\tau)\frac{1}{\tau^2} \exp\left(-r^2/(4k\tau)\right)d\tau \tag{4.2}$$

In general (4.1) and (4.2) has to be solved by numerical quadrature. A considerable saving in calculation time can be obtained by splitting up the integration in two parts. One - usually small -

part in which the exponential has to be calculated and one where it can be assumed equal to unity ($4k\tau > 10\ r^2$). In the computer program PSAMA the numerical quadrature is performed by the standard procedure. RISOE/ADAPINT/A B6700.

## 5. THE TIME DECAY OF THE HEAT SOURCE

The time dependence of q(t) can be taken into account through different expressions.

In ref.(5) is used an expression

$$q(t) = q_o \left(\frac{t_c+t}{t_c}\right)^x \qquad (5.1)$$

Where $t_c$ is the cooling time of the waste, $q_o$ the source strength at the deposition time and x an exponent used to fit q(t) to the actual experimental or theoretically calculated time dependence of the heat production in the waste.

A probably more realistic expression fitted to the decay heat calculations performed in ref.(10)adjusted to 30 years cooling time is

$$\begin{aligned} q(t) &= q_o \cdot \exp(-0.0133 \cdot t) \quad 0 \leq t \leq 170 \text{ years} \\ &= 0.13918 \cdot q_o \cdot \exp(-0.0017 \cdot t) \quad t > 170 \text{ years} \end{aligned} \qquad (5.2)$$

The transition to other cooling times is obvious.

## 6. CHOICE OF CONSTANTS

The choice of constants which are necessary to obtain actual numerical results is far from unique. The quantity $D_o(T)$ in (2.1) may be calculated according to formula (10) in ref. (1), but the constants quoted are only given for KCl at one temperarure In the same paper the great spread in the value $K_o$ is postulated presumably because of the random number of dislocations which are crossed by the surface of the brine inclusion.

In ref. (3) a semilogarithmic plot of $D_o(T)$ for rock salt is given which corresponds to the expression

$$D_o(T) := 10^{-4} \times \exp(0.016(T-92.5)) \text{ m/år/}(^{o}C/m) \qquad (6.1)$$

This plot is derived from conservative estimate of experimental values reported in ref.(7). In a later report ref.(6) an estimate of the same data leads to the formula

$$\log(10^4 \cdot D_o) = 0.00656 \cdot T - 0.6036$$

$$D_o = 10^{-4} \exp(0.015105 \cdot (T - 92)) \qquad (6.2)$$

an expression practically identical with (6.1).

Expressions (4.1) and (4.2) can only be used if $\lambda$ and $k$ is assumed independend of $r$ and $T$.

In ref.(4) graphs are shown of $k$ and $\lambda$ which demonstrate strong dependence of the temperature. Such dependence is outside the scope of the present treatment, where fixed values of $k$ and $\lambda$ have to be used. The influence of $k$ and $\lambda$ values on the temperatures calculated by (4.1) is such, that the higher temperatures are assumed by the determination of $k$ and $\lambda$ values the higher the temperatures calculated by (4.1) becomes.

The Graphs in ref.(4) are based on measurements reported by F. Birch in ref.(8). As pointed out by Birch the inverse value $1/\lambda$ comes very close to a linear function of temperature. The temperature dependence of $\lambda$ and k is very well approximated by the expressions

$$\lambda = 31.536/(7.2\cdot10^{-4}T + 0.155) \text{ MJ/year/m/}^{o}\text{C} \tag{6.3}$$

$$k = \lambda/(\rho c) = \lambda/1.95 \text{ m}^2\text{/year} \tag{6.4}$$

In the following $\lambda$ and k are calculated by these formula unless other values are directly quoted.

## 7. NUMERICAL SOLUTION

The numerical solution of (3.1) or (3.2) based upon the solutions of (4.1) and (4.2) is performed by the standard procedure RISOE/DIFSUB/A B6700 in the program PSAMA.

In order to check the method, comparisons are made with approximate solutions under certain simplifying conditions which can be calculated by hand. These comparisons serve at the same time to assess the influence of the temperature dependence of the diffusion coefficient $D_o$ and the time dependence of the heat source.

The migration speed increases with rising temperature, so to be on the safe side, but not too far, by calculating the brine migration the temperature used to determine k and $\lambda$ should be equal to the maximum temperature calculated with (4.1) at $r=r_o$. This can be achieved by a few trial and error attempts.

Approximate solutions for the brine in-flow are derived in Appendix I and II for the cases where $D_o$ is constant, $K_o = 0$ and the exponent in the source expression (5.1) respectively takes the values $x = 0$ (constant source) and $x = -1$.

In Table (7.1) these results are compared with numerical calculations of the same cases performed with PSAMA as well as with the PSAMA result when 6.1 is used.

In these calculations the following values have been used

$k = 51.5\ m^2/year$
$\lambda = 98.2\ MJ/m/^oC/year$
$\sigma = 5\ liter/m^3$
$q_o = 10512\ MJ/m/year$
$r_o = 0.2\ m$

The k- and $\lambda$-value corresponds to a salt temperature of $200^oC$ according to ref. (3) and (4). $q_o$ and $r_o$ are the values quoted in ref.(5).

Table 7.1.

| $t_o$ years | accumulated brine inflow liters/m | | | | | |
|---|---|---|---|---|---|---|
| | $x=0;\ D_o=10^{-4}$ | | $x=-1;\ D_o=10^{-4}$ | | $x=-1;\ D_o$ from | $x=-1$ |
| | Formula AI.5 | PSAMA | Formula AII.2 | PSAMA | formula (6.1) PSAMA | $D_o=3.91\ 10^{-5}$ formula AII.2 |
| 1 | 0.0535 | 0.0529 | 0.0526 | 0.0521 | 0.0293 | 0.0205 |
| 2 | 0.1075 | 0.1061 | 0.1036 | 0.1031 | 0.0627 | 0.0403 |
| 5 | 0.2676 | 0.2666 | 0.2475 | 0.2466 | 0.1617 | 0.0963 |
| 10 | 0.5352 | 0.5341 | 0.4619 | 0.4619 | 0.3045 | 0.1797 |
| 20 | 1.0746 | 1.0681 | 0.8202 | 0.8226 | 0.5771 | 0.3191 |
| 50 | 2.6762 | 2.6689 | 1.5749 | 1.5774 | 0.8754 | 0.6128 |
| 100 | 5.3552 | 5.3451 | 2.3545 | 2.3584 | 1.1623 | 0.9161 |
| 200 | 10.7468 | 10.6968 | 3.2706 | 3.2803 | 1.4434 | 1.2726 |
| 500 | 26.7617 | 26.7491 | 4.6111 | 4.6264 | 1.7942 | 1.7942 |

Very good agreement is found between results from formulas A1.5, AII.2 and the corresponding PSAMA results.

The PSAMA results with temperature dependend diffusion coefficient (6.1) in collumn 5 can be compared with the results in collumn 6 from formula AI.2 where $D_o$ has been changed so as to obtain agreement at $t_o$=500 years.

Similar results may be obtained for the outward movement of vapour containing brine inclusions. Formulas analogue to the ones derived in APPENDIX II can be obtained by systematic exchange of $t_o$-s with t on the right sides and s with t on the left sides in APPENDIX II. This leads to the following expression for the distance, r(t) reached at time t, when $r(0)=r_o$

$$r(t) = \sqrt{r_o^2 + \frac{D_o q_o t_c}{\pi\lambda} \ln\left(\frac{t_c+t}{t_c}\right)} \tag{7.1}$$

In Table 7.2 values obtained by this formula are compared with values calculated by PSAMA.

The material constants are the same as quoted above. x is set equal to -1 and $D_o=6.748\ 10^{-2}\ m^2/year/^oC$ is calculated by use of formula (13) and constants found in Table 2 of ref. (2).

Table 7.2

| t years | radial distance r(t) | |
|---|---|---|
| | Formula (7.1) m | PSAMA m |
| 0 | 0.2 | 0.2 |
| 1 | 1.521 | 1.521 |
| 2 | 2.124 | 2.117 |
| 5 | 3.275 | 3.260 |
| 10 | 4.471 | 4.453 |
| 20 | 5.955 | 5.941 |
| 50 | 8.250 | 8.253 |
| 100 | 10.086 | 10.109 |
| 200 | 11.887 | 11.929 |
| 1000 | 15.661 | 15.724 |

Finally in Fig. 7.1 is shown the time dependent temperature field corresponding to the solution of the two last collumns of Table 7.1 and of Table 7.2. The temperatures are calculate by use of (4.1) in the program TEMPLI.

## 8. COMPARISON WITH EXPERIMENT

Very few in situ experiments with brine migration in rock salt has been performed. The only available experimental material with which to compare the mathematical model is measurements carried out under Project Salt Vault (PSV) reported in ref.(4).

Several problems appear , when the results of these measurements are assessed. One important problem is how to take account of the particular geometrical configuration of the heat source, which consists of 7 line sources 6' long arranged in a regular hexagonal array with one line source in the centre.

The first step was to calculate the temperature field around this configuration, which could be made by superposition of the Green functions of finite linesources by help of the program BCHM. In Fig. 8.1 comparison is made between results from BCHM and from an apparently identical type of calculations in PSV reported on page 22 in ref.(4). In both calculations the same source strength and salt data corresponding to 100$^{o}$C has been used. The agreement is quite convincing.

The next step was to reconstruct the measured temperature distribution found by measurements in the brine migration experiment. In Fig.8.2, p.16 is given a reproduction from PSV showing the temperatures measured in a number of points and in paranthesis is shown the corresponding temperatures calculated by BCHM.

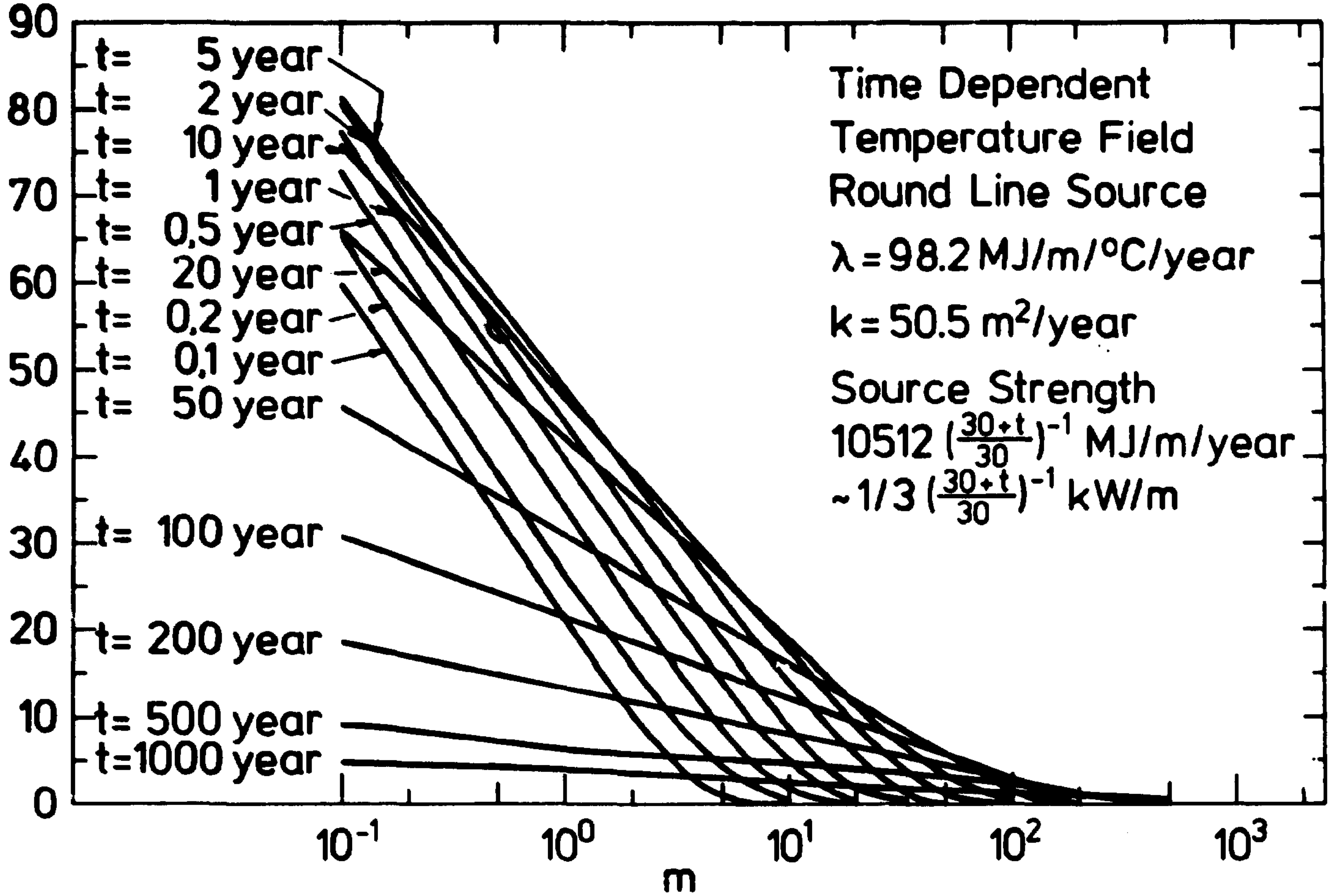
TEMPERATURE (°C)
90
80
70
60
50
40
30
20
10
0
t= 5 year
t= 2 year
t= 10 year
t= 1 year
t= 0,5 year
t= 20 year
t= 0,2 year
t= 0,1 year
t= 50 year
t= 100 year
t= 200 year
t= 500 year
t=1000 year
Time Dependent
Temperature Field
Round Line Source
λ = 98.2 MJ/m/°C/year
k = 50.5 m²/year
Source Strength
10512 ((30+t)/30)⁻¹ MJ/m/year
~1/3 ((30+t)/30)⁻¹ kW/m
10⁻¹
10⁰
10¹
10²
10³
m

Fig. 7.1

There is some uncertainty in the reporting of the experiment. The power input has been subject to small variations and short interruptions. However as recommended in Table 2 in ref. (6) the power input can be assumed 11 kW total in 430 days and 15 kW the last 150 days. When this power input is used in BCHM with 100°C salt data the temperature becomes far higher than the ones measured. It seems that PSV have encountered the same problems, since it is remarked in connection with Fig. 11.19. on page 178 that the (well agreeing) theoretical curve "is calculated with 20°C thermal properties rather than the 100°C properties used for previous calculations". All this may at least partially be explained by escape of heat up through the floor of the cave (Room 1 or 4), from which the experimental holes are drilled. Another extra cooling effect may be the airflow used to collect the water component of the brine.

As shown below the temperature at the hole wall plays an important role in assessing the brine inflow. Data corresponding to ambient temperature, 23°C is chosen for the BCHM calculation in order to get the best agreement with measured temperatures. As is seen from the Fig. 4 the agreement is quite good in the vicinity of the central hole.

The next step consists in evaluating the influence of the source configuration on the brine flow $\vec{B}$. This is defined

$$\vec{B} = \sigma \vec{V} \ L/m^2/\text{Year} \tag{8.1}$$

when $\sigma$ is the brine density in $L/m^3$. Using only the first term in (2.1) we get

$$\vec{B} = \sigma D_o(T) \nabla T \tag{8.2}$$

The brine flow is always directed along the temperature gradient and the heat flow defined as

$$\vec{J} = -\lambda (T) \nabla T \tag{8.3}$$

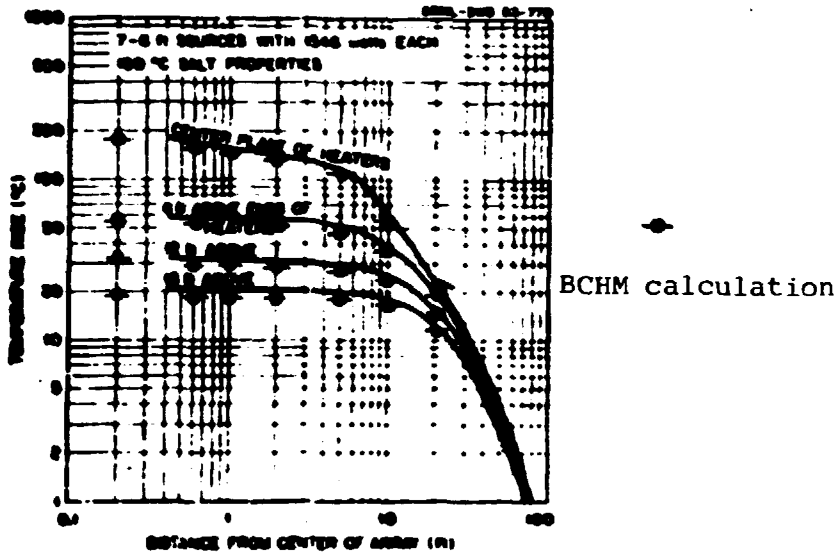


Fig. 3.8. Temperature Rise Profile in Demonstration Array Along Radial Between Peripheral Heaters After 1½ Years.

Fig. 8.1

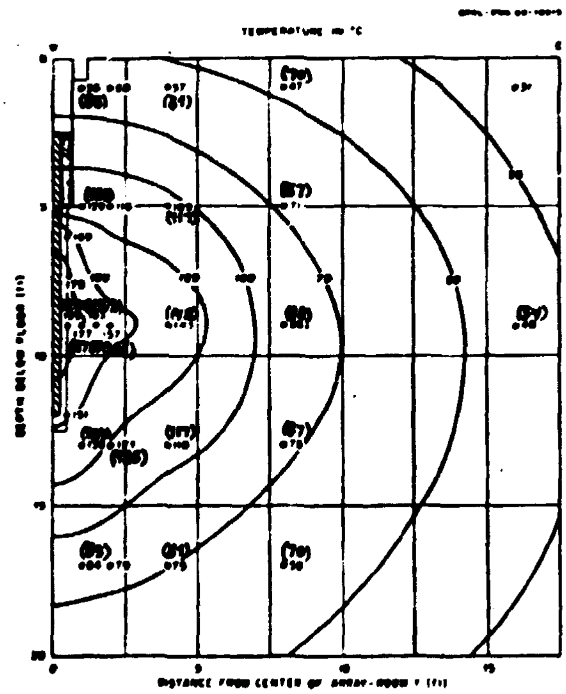

Fig. 11.13. Temperature Contours in Vertical Plane – East-West Direction, Room I.

Fig. 8.2

Assuming spatialy constant density $\sigma = \sigma_o$ the inflow of brine, bf into an isothermal, closed surface, S round a heat source, q(t) becomes

$$bf = -\int_S \vec{B}.\vec{ds} = -\int_S \sigma_o D_o(T)\nabla T.\vec{ds}$$

$$= \int_S \frac{\sigma_o D_o(T)}{\lambda(T)} \vec{J}.\vec{ds} = \frac{\sigma_o D_o(T)}{\lambda(T)} q(t) \qquad (8.4)$$

If $D_o(T)$ and $\lambda(T)$ are constants then total in leakage, BF is obtained by integration with respect to time.

$$BF(t) = \int_0^t bfd\tau = \frac{\sigma_o D_o}{\lambda} \int_0^t q(\tau)d\tau \qquad (8.5)$$

This formula is covering the results both in APPENDIX I and II.

*In real life both* $\lambda$ *and particularly* $D_o$ is strongly temperature dependend. However if $\sigma$ remains fairly constant in space and time, if the isothermal surface remains such although changing temperature and if its temperature is known as function of time then BF may be given as

$$BF(t) = \sigma_o \int_0^t \frac{D_o(T(\tau))}{\lambda(T(\tau))} q(\tau)d\tau \qquad (8.6)$$

It is worth while to note that under these circumstances BF is independend of the actual shape of the source.

In Appendix III the variation of $\sigma$ with time is investigated in a relevant case yilding the result that $\sigma$ remains fairly constant inside the time scale of the PSV experiment.

On this background it would be tempting, since the exact shape of the source seems less important, to apply PSAMA directly on the PSV experiment just taking the PSAMA-inflow on the summed up length of the seven line sources.

However (8.6) illustrates that the way in which the temperature varies may play an important role in the calculation of BF.

The difference between the wall temperature from an infinite line source and that of the central hole of the finite PSV-array is illustrated in Table 8.1 where the temperatures on the wall of the hole is given as function of time. One difference is that the temperature round an infinite source, constant in time continues to increase, whereas the temperature round a finite array levels off towards a steady state value. The shape of the temperature growth will thus be different. In order to obtain the same final temperature just before the heaters are shut down and the brine inflow finally measured, $100^{o}C$ salt data has to be used in the infinite linear case. The linear power per unit length is the same in both cases and given in Table 8.1. Finally the value of BF per unit length is given for both cases calculated by (8.6) and for the infinite line source also directly by PSAMA

Table 8.1

| Time | Source strength | BCHM | | TEMPLI-PSAMA | | |
|---|---|---|---|---|---|---|
| | | wall temp. | BF from(8.6) | wall temp. | BF from(8.6) | BF PSAMA |
| Years | MJ/m/y | $^{o}C$ | liter/m | $^{o}C$ | liter/m | liter/m |
| 0 | 26787 | 23.0 | 0.0 | 23.0 | 0.0 | 0.0 |
| 0.1 | - | 134.1 | 0.012 | 123.3 | 0.010 | 0.012 |
| 0.2 | - | 141.9 | 0.034 | 133.9 | 0.029 | 0.029 |
| 0.5 | - | 148.9 | 0.111 | 148.0 | 0.100 | 0.091 |
| 1.0 | - | 152.5 | 0.253 | 158.6 | 0.250 | 0.209 |
| 1.178 | 26787 | 153.2 | 0.306 | 161.1 | 0.310 | 0.253 |
| 1.178 | 36528 | 153.2 | 0.306 | 161.1 | 0.310 | 0.253 |
| 1.589 | 36528 | 199.6 | 0.587 | 210.9 | 0.646 | 0.510 |

In the already quoted Tabel 2. of ref.(6) the data and the results of the two practically identical PSV-experiments in Room 1 and Room 4 have been concentrated, probably after some evaluation, since the reporting in ref.(4) is somewhat opaque.

The value of brine content in the salt quoted corresponds to $\sigma = 5L/m^3$ and the length of the heaters is given as 1.85 m. Two values of total brine inflow BF are quoted for each experiments, one during the heating period which is quite small and one after, which is roughly ten times greater.

The total amount of BF quoted is probably the one with which the results in Table 8.1 should be compared. The final values in collumn 4, 6 and 7 should be multiplied by 7 x 1.85 in order to compare as follows

| | Total brine inflow liter |
|---|---|
| Room 1 experiment | 10.7 |
| Room 4 experiment | 13.6 |
| BCHM (col.4) calcul.by(8.6) | 7.6 |
| TEMPLI (col.6) calcul.by(8.6) | 8.36 |
| PSAMA (col.7) calcul. | 6.59 |

It should be remembered that the PSV-report ref.(4) leaves a considerable uncertainty with regard to the precise circumstances of the experiments e.g. the composition of the salt and the way the brine inflow has been monitored.

Consequently the comparison above should be treated with a certain reservation. For instance if BCHM is used with the 100$^\circ$C salt data recommended early in ref.(4) the inflow according to formula (8.6) comes out with 16.6 liters which should be compared with 7.6 liters as quoted above.

Regarding the comparison between the results of different theoretical calculations shown in Table 8.1 the values calculated by (8.6) are taking the temperature dependence of $\lambda$ into consideration, whereas direct PSAMA calculation uses fixed $\lambda$-value. The two sets which ought to be directly comparable are in column 6 and 7.

It is hard to determine, which of the methods used in culumn 6 and 7 is the most exact. Although the temperature dependence is taken into account in formula (8.6), the temperatures used are still obtained by assuming fixed, $100^{\circ}C$ salt data. Added to this comes the uncertainty of changes in time and space of $\sigma$. According to Table AIII.1 $\sigma$ is decreasing, so formula (8.6) is an overestimate. If $\sigma$ is multiplied by the values of $\sigma/\sigma_0$ from this table we get the following version of the two last columns in Table 8.1

| Time<br>Year | (8.6) with corrected $\sigma$<br>liter/m | PSAMA<br>liter/m |
|---|---|---|
| 0.0 | 0.0 | 0.0 |
| 0.1 | 0.010 | 0.012 |
| 0.2 | 0.028 | 0.029 |
| 0.5 | 0.096 | 0.091 |
| 1.0 | 0.226 | 0.209 |
| 1.178 | 0.275 | 0.253 |
| 1.589 | 0.550 | 0.510 |

According to the reasoning in Appendix III, last paragraph, This correction should result in an underestimation. However several other assumptions are introduced in the derivation of (8.6), e.g. that the heat accumulated or extracted inside the surface S in (8.4) is negigible. For a steady line source, where the temperature continues to rise overall, this condition cannor be said to be completely complied with.

As demonstrated in ref.(9) a rather good representation of the temperature distribution can be obtained by use of suitable, fixed salt data. When this is the case, the direct migration method developed in section 3 and 4 and incorporated in PSAMA for infinite line sources should lead to a near exact result.

For other source shapes, with the exeption of point sources, this method is hardly feasible, and in such cases formula (8.6) comes in handy as an estimate.

REFERENCES

(1) T.R. Anthony and H.E. Cline, The Thermal Migration of Liquid Droplets through Solids. Journal of Applied Physics, Vol. 42, No. 9, pp. 3380-87, 1971.

(2) T.R. Anthony and H.E. Cline, The Thermo-migration of Biphase Vapour-Liquid Droplets in Solids. Acta Metallurgica , Vol. 20, pp. 247-55, 1972.

(3) G.H. Jenks, - Radiolysis and Hydrolysis in Salt-Mine-Brines ORNL-TM-3717, March 1972.

(4) R.L. Bradshaw and W.C. McClain, Project Salt Vault: A Demonstration of the Disposal of High-Activity Solidified Waste in Underground Salt Mines. ORNL-4555, April 1971.

(5) Disposal of High-Level Waste from Nuclear Power Plants in Denmark. Elkraft and Elsam. July 3rd, 1978.

(6) G.H. Jenks, Effects of Temperature Gradients Stress, and Irradiation on Migration of Brine Inclusions in Salt Repository. ORNL 5526, July 1979.

(7) R.L. Bradshaw and F. Sanchez, Brine Migration Studies. Health Phys. Div. Annu. Prog. Rep. July 31, 1968. ORNL 4316 p. 32.

(8) Francis Birch and J. Clark, The Thermal Conductivity of Rocks and Its Dependence on Temperature and Composition. Am. J. Sci 238, 529-58, 613-35 (1940).

(9) H. Neltrup, Temperature Field Around Waste Calculated by Use of Green Functions. Private Communication, RP-16-79.

(10) C.F. Højerup, Calculation of Power Generation and Radiation Levels in Nuclear Waste Material. Private Communication. RP-17-79.

APPENDIX I

In the case where $D_o(T)$ and $q(t)$ are constants, and $K_o=0$, equation (3.2) takes the form

$$\frac{dr}{ds} = \frac{D_o q_o r}{8\pi\lambda k}\int_0^{t_o-s} \frac{1}{\tau^2} \exp\,(-r^2/(4k\tau))\,d\tau \qquad \text{(AI.1)}$$

substituting $x = \frac{1}{\tau}$, $dx = \frac{-d\tau}{\tau^2}$ we get

$$\frac{dr}{ds} = \frac{D_o q_o r}{8\pi\lambda k}\int_{1/(t_o-s)}^{\infty} \exp\,(-x\, r^2/(4k))\,dx$$

$$= \frac{D_o q_o}{2\pi\lambda}\,\frac{1}{r}\,\exp\,(-\,r^2/(4k(t_o-s))) \qquad \text{(AI.2)}$$

Within the migration range which we work here, $r^2/(4k)$ will be of the order of $10^{-2}$ year so we may assume that the exponent in (AI.2) is unity except when $t_o$-s is of the order $10^{-2}$ year. Accordingly

$$\frac{dr}{ds} \approx \frac{D_o q_o}{2\pi\lambda}\,\frac{1}{r}\;; \qquad \frac{dr^2}{ds} = \frac{D_o q_o}{\pi\lambda}$$

$$r^2(s) = \frac{D_o q_o}{\pi\lambda}\; s + c \qquad \text{(AI.3)}$$

the initial condition $r(0) = r_o$ leads to

$$r^2(t_o) = \frac{D_o q_o}{\pi\lambda}\, t_o + r_o^2 \qquad \text{(AI.4)}$$

Assuming a brine density, $\sigma$ the total brine inflow BF in time $t_o$ become

$$BF = \sigma \cdot \pi \cdot (r^2(t_o) - r_o^2) = \sigma\,\frac{D_o q_o}{\lambda}\, t_o \qquad \text{(AI.5)}$$

# APPENDIX II

The case with temperature independent diffusion coefficient (3.2) takes the form

$$\frac{dr}{ds} = \frac{D_o r}{8\pi\lambda k}\int_0^{t_o-s} q(t_o-s-\tau)\,\frac{1}{\tau^2}\,\exp\,(-r^2/(4k\tau))d\tau \qquad \text{(AII.1)}$$

Within the short range of migration considered here, we can define a short time interval $\Delta t$ such that $r^2/(4k\Delta t) = 0.01$, $\exp\,(-r^2/4k\Delta t) \sim 1-0.01=0.99$.

The following approximation is then introduced

$$\frac{dr}{ds} \simeq \frac{D_o r}{8\pi\lambda k}\,\left(\int_0^{\Delta t} q(t_o-s)\frac{1}{\tau^2}\,\exp(-r^2/(4k\tau))d\tau + \int_{\Delta t}^{t_o-s} q(t_o-s-\tau)\,\frac{d\tau}{\tau^2}\right.$$

$$= \frac{D_o r}{8\pi\lambda k}\,\left(q(t_o-s)\,\frac{4k}{r^2}\,\exp\,(-r^2/(4k\Delta t)\,+\int_{\Delta t}^{t_o-s} q(t_o-s-\tau)\,\frac{d\tau}{\tau^2}\right)$$

$$= \frac{D_o r}{8\pi\lambda k}\,\left(q(t_o-s)\left(\frac{4k}{r^2} - \frac{1}{\Delta t}\right) + \int_{\Delta t}^{t_o-s} q(t_o-s-\tau)\,\frac{d\tau}{\tau^2}\right)$$

We now specialize to (5.1) with x=-1 and obtain

$$\frac{dr}{ds} = \frac{D_o r}{8\pi\lambda k}\,\left(\frac{t_c q_o}{t_c+t_o-s}\left(\frac{4k}{r^2} - \frac{1}{\Delta t}\right) + q_o\int_{\Delta t}^{t_o-s} \frac{t_c}{\tau^2(t_c+t_o-s-\tau)}\,d\tau\right)$$

$$= \frac{D_o r}{8\pi\lambda k}\,\frac{q_o t_c}{t_c+t_o-s}\,\left(\frac{4k}{r^2} - \frac{1}{\Delta t} + \int_{\Delta t}^{t_o-s}\left(\frac{1}{\tau^2} + \frac{1}{t_c+t_o-s}\left(\frac{1}{\tau} + \frac{1}{t_c+t_o-s-\tau}\right)d\tau\right)\right.$$

$$= \frac{D_o r}{8\pi\lambda k}\,\frac{q_o t_c}{t_c+t_o-s}\left(\frac{4k}{r^2} - \frac{1}{t_o-s} + \frac{1}{t_c+t_o-s}\left(\ln\left(\frac{t_o-s}{\Delta t}\right)-\ln\left(\frac{t_c-t_o-s-\Delta t}{t_c}\right)\right)\right))$$

As long as $t_o-s>\Delta t$ the first term inside the paranthesis will dominate leading to the approximation

$$\frac{dr}{ds} \simeq \frac{D_o}{2\pi\lambda}\,\frac{1}{r}\,\frac{q_o t_c}{t_c+t_o-s}$$

$$r^2 \;= \frac{-D_o}{\pi\lambda}\, q_o\; t_c\; \ln(t_c+t_o-s) \;+\; c$$

$$s = 0 \Rightarrow r = r_o$$

$$c = r_o + \frac{D_o t_c q_o}{\pi\lambda}\;\; \ln(t_c + t_o)$$

$$r^2(s) \;=\; r_o^2 + \frac{D_o t_c q_o}{\pi\lambda}\, \ln\, \left(\frac{t_c+t_o}{t_c+t_o-s}\right)$$

in leakage at time $t_o$

$$BF= \pi\cdot\sigma(r^2(t_o)-r_o^2) \;=\; \sigma\,\frac{D_o q_o}{\lambda}\; t_c\; \ln\, \left(\frac{t_c+t_o}{t_c}\right) \qquad \text{(AII.2)}$$

It is interesting to note that the precise value of k does not enter into the approximations (AI.5) and (AII.2), whereas the order of magnitude of k as we have seen is determining for their validity.

## APPENDIX III

The time dependend spatial distributional of the brine density, $\sigma$ is obtained by the simultanious solution of the heat conduction equation

$$\nabla^2 T = \frac{1}{k}\frac{\partial T}{\partial t} \qquad \text{(AIII.1)}$$

and the equations determining the brine flow $\vec{B}$

$$\vec{B} = \sigma(r,t)\hat{V} = \sigma(r,t)\ D_o \nabla T \qquad \text{(AIII.2)}$$

$$\begin{aligned}\frac{\partial\sigma}{\partial t} &= -\ \nabla\vec{B} = -\nabla(\sigma D_o \nabla T)\\ &= -D_o\nabla\sigma\cdot\nabla T - \sigma\frac{dD_o}{dT}(\nabla T)^2 - \sigma D_o\ \nabla^2 T\end{aligned} \qquad \text{(AIII.3)}$$

By insertion of (AIII.1)

$$\frac{\partial\sigma}{\partial t} = -\ D_o\ \nabla\sigma.\nabla T - \sigma\frac{dD_o}{dT}(\nabla T)^2 - \frac{\sigma D_o}{k}\frac{\partial T}{\partial t} \qquad \text{(AIII.4)}$$

The initial condition is $\sigma(r,t) = \sigma_o$ and consequently $\nabla\sigma = 0$ for $t = 0$; so we start by neglecting the first term. The ensuing ordinary differential equation can then be solved in the following closed form

$$\begin{aligned}\sigma &= \sigma_o \exp\left(-\int_0^t \left(\frac{dD_o}{dt}(\nabla T)^2 + \frac{D_o}{k}\frac{dT}{d\tau}\right) d\tau\right.\\ &= \sigma_o \exp\left(-\int_0^t \frac{dD_o}{dt}(\nabla T)^2\, d\tau - \int_{T(0)}^{T(t)} \frac{D_o(T)}{k(T)}\, dT\right)\end{aligned} \qquad \text{(AIII.5)}$$

Specializing (AIII.5) to the case, where $D_o$ does not depend on temperature, the first integral disappears. Assuming further more that k is a constant, (AIII.6) takes the form

$$\sigma = \sigma_o \exp(- \frac{D_o}{k} (T(t) - T(0)) =$$

within the scope of this investigation $T(t) - T(0) \leq 200^oC$ and

$$\frac{D_o}{k} = \frac{5 \cdot 10^{-4}}{50} = 10^{-5}$$

are reasonable upper limits giving

$$\sigma_{min} = \sigma_o \exp(2 \cdot 10^{-3}) \simeq \sigma_o (1 - 2.10^{-3})$$

under these circumstances $\sigma$ will remain very close to $\sigma_o$ everywhere and $\nabla\sigma =$ ' indeed a good approximation.

However when a temperature dependence as given in (6.1) is assumed for $D_o$, the first term in (AIII.5) becomes dominating. In order to evaluate its value an expression for $\nabla T$ has to be introduced.

Assuming that the brine leakage is studied on a closed surface, S as close to the heat source as possible that, although changing temperature, remains isothermal in space, then we have

$$\nabla T = \frac{q}{S} \frac{1}{\lambda} \qquad \text{(AIII.6)}$$

wh·re q/S is the heat flux per unit area.

When $D_o$ is expressed by (6.1) and $k(T)$ by (6.2) and (6.3) the second integral in (AIII.5) can be calculated by analytical methods.

The first integral in (AIII.5) may be solved numerically when the q and T is known for a number of t-values.

In Table AIII.1 numerical evaluation of (AIII.5) is made for the cylinder symetrical case corresponding to Table 8.1.

Table AIII.1

| t years | q MJ/m | T $^{o}C$ | $\sigma/\sigma_o$ formula (AIII.5) |
|---|---|---|---|
| 0 | 26687 | 23 | 1.0 |
| 0.1 | 26687 | 123.3 | 0.999 |
| 0.2 | 26687 | 133.9 | 0.980 |
| 0.5 | 26687 | 148.0 | 0.928 |
| 1.0 | 26687 | 158.6 | 0.824 |
| 1.178 | 26687/36528 | 161.1 | 0.786 |
| 1.598 | 36528 | 210.9 | 0.526 |

It is seen that $\sigma$ remains fairly constant, although gradually decreasing, till the moment where the power is increased (by a factor of 15/11).

It should be pointed out that as soon as $\sigma$ starts decreasing the first term on the left in (AIII.4) will start counteracting, since $\nabla\sigma$ and $\nabla T$ will have oposite signs. Tentatively the conclusion may be expressed that $\sigma$ will not vary too much inside a few years in case of moderately concentrated heat sources.

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Abstract

A mathematical model for the brine migration in rock salt around an infinite line heat source is set up. The temperature field around the time dependent heat source is calculated by use of Green functions. Numerical solutions are obtained by the computer program PSAMA and results are compared with hand calculations for certain simple cases.

By general considerations of the migration field approximate values of the brine inflow, which are independent of the source shape, is obtained and these results are used to estimate the agreement with the experimental results from Project Salt Vault.

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